METHOD FOR FRAGMENT PREPARATION

ABSTRACT

A method for characterizing a molecular fragment to collect data related to the fragment that allows its evaluation for drug discovery purposes. Starting with a two-dimensional model of the fragment, an initial three-dimensional model of the fragment is derived. Conformers of the fragment are identified. The conformers are then clustered, and a representative conformer is selected from each cluster. An *ab initio* or semi-empirical calculation and analysis is performed on one or more of the selected conformers. Each atom in the selected conformer is then assigned a type. The selected conformer is analyzed to determine if it is structurally symmetric. If so, the three-dimensional model of the fragment is adjusted to reflect the symmetry. The size of the fragment is calculated to allow geometric analysis of how the fragment physically fits with the protein and/or other fragments. The solvation energy of the fragment is calculated. The free energy curve for the fragment is calculated. Derivatization points for the fragment are then determined; a score is then assigned to each derivatization point, reflecting the ease or difficulty in bonding at the derivatization points. The fragment is then assigned a name and categorized. The fragment and its data derived in the above process can then be stored in a database.